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3 SEP 2002

03SEP02 E745445-2 D01063  
P01/7700 0.00-0220438.6

3. Full name, address and postcode of the or of each applicant (underline all surnames)

University of Warwick  
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Patents ADP number (if you know it)

If the applicant is a corporate body, give the country/state of its incorporation

United Kingdom

798553001

4. Title of the invention

"Formation of Lattice-Tuning Semiconductor Substrates"

5. Name of your agent (if you have one)

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"Address for service" in the United Kingdom to which all correspondence should be sent (including the postcode)

4220 Nash Court  
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United Kingdom

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7271125001

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12. Name and daytime telephone number of person to contact in the United Kingdom

Richard Harding  
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## "Formation of Lattice-Tuning Semiconductor Substrates"

This invention relates to the production of lattice-tuning semiconductor substrates, and is more particularly, but not exclusively, concerned with the production of relaxed SiGe (silicon/germanium) "virtual substrates" suitable for the growth of strained silicon or SiGe active layers and unstrained III-V semiconductor active layers within which active semiconductor devices, such as MOSFETs, may be fabricated.

It is known to epitaxially grow a strained Si layer on a Si wafer with a relaxed SiGe buffer layer interposed therebetween, and to fabricate semiconductor devices, such as MOSFETs, within the strained Si layer in order to enhance the properties of the semiconductor devices. The buffer layer is provided in order to increase the lattice spacing relative to the lattice spacing of the underlying Si substrate, and is generally called a virtual substrate.

It is known to epitaxially grow an alloy of silicon and germanium (SiGe) on the silicon substrate to form the buffer layer. Since the lattice spacing of SiGe is greater than the normal lattice spacing of Si, the desired increase in lattice spacing is achieved by the provision of such a buffer layer if the buffer layer is allowed to relax.

The relaxation of the buffer layer inevitably involves the production of dislocations in the buffer layer to relieve the strain. These dislocations generally form a half loop from the underlying surface which expands to form a long dislocation at the strained interface. However the production of threading dislocations which extend through the depth of the buffer layer is detrimental to the quality of the substrate, in that such dislocations can produce an uneven surface and can cause scattering of electrons within the active semiconductor devices. Furthermore, since many dislocations are required to relieve the strain in a SiGe layer, such dislocations inevitably interact with one another causing pinning of threading dislocations. Additionally more dislocations are required for further relaxation, and this can result in a higher density of threading dislocations.

Known techniques for producing such a buffer layer, such as are disclosed in US5442205, US 5221413, WO 98/00857 and JP 6-252046, involve linearly grading the Ge composition in the layer in order that the strained interfaces are distributed over the graded region. This means that the dislocations that form are also distributed over the graded region and are therefore less likely to interact. However such techniques suffer from the fact that the main sources of dislocations are multiplication mechanisms in which many dislocations are generated from the same source, and this causes the dislocations to be clustered in groups, generally on the same atomic glide planes. The strain fields from these groups of dislocations can cause the virtual substrate surface to have large undulations which is both detrimental to the quality of the virtual substrate and has the added effect of trapping threading dislocations.

US 2002/0017642A1 describes a technique in which the buffer layer is formed from a plurality of laminated layers comprising alternating layers of a graded SiGe layer having a Ge composition ratio which gradually increases from the Ge composition ratio of the material on which it is formed to an increased level, and a uniform SiGe layer on top of the graded SiGe layer having a Ge composition ratio at the increased level which is substantially constant across the layer. The provision of such alternating graded and uniform SiGe layers providing stepped variation in the Ge composition ratio across the buffer layer makes it easier for dislocations to propagate in lateral directions at the interfaces, and consequently makes it less likely that threading dislocations will occur, thus tending to provide less surface roughness. However this technique requires the provision of relatively thick, carefully graded alternating layers in order to provide satisfactory performance, and even then can still suffer performance degradation due to the build-up of threading dislocations.

It is an object of the invention to provide a method of forming a lattice-tuning semiconductor substrate in which performance is enhanced by decreasing the density of threading dislocations as compared with known techniques.

According to the present invention there is provided a method of forming a lattice-tuning semiconductor substrate, comprising:

(a) defining parallel strips of a Si surface by spaced parallel isolating means;

5 (b) selectively growing a first SiGe layer on the strips such that first dislocations extend preferentially across the first SiGe layer between the isolating means to relieve the strain in the first SiGe layer in directions transverse to the isolating means; and

10 (c) growing a second SiGe layer on top of the first SiGe layer to overgrow the isolating means such that second dislocations form preferentially within the second SiGe layer above the isolating means to relieve the strain in the second SiGe layer in directions transverse to the first dislocations.

15 It is believed that such a technique is capable of producing high quality SiGe virtual substrates with extremely low levels of threading dislocations, that is with levels from less than  $10^6$  dislocations per  $\text{cm}^2$  to virtually no threading dislocations. This is as a result of the fact that dislocations are produced which serve to relax the SiGe material in two mutually transverse directions whilst being spatially separated so that the two sets of dislocations cannot interact with one another in such a manner as to produce  
20 threading dislocations extending through the depth of the SiGe material.

As a result a thinner virtual substrate can be produced for a given Ge composition with both the threading dislocation density and the surface undulations being very greatly reduced. This results in a virtual substrate which is superior and  
25 allows power to be more readily dissipated. The decrease in roughness of the surface of the virtual substrate renders further processing more straightforward in that polishing of the surface can be minimised or dispensed with altogether, and loss of definition due to unevenness of the surface is minimised. The quality of the virtual substrate produced may be such as to render it suitable for specialised applications, for example in  
30 microelectronics or in full CMOS integration systems.

In order that the invention may be more fully understood, reference will now be made to the accompanying drawings, in which:

Figure 1 is an explanatory view showing the effect of the transverse dislocations  
5 in preventing relaxation of a strained Si substrate in the longitudinal direction; and

Figure 2 shows successive steps in a method of forming a lattice-tuning semiconductor substrate in accordance with the invention.

10 The following description is directed to the formation of a virtual lattice-tuning Si substrate on an underlying Si substrate with the interposition of a SiGe buffer layer. However it should be appreciated that the invention is also applicable to the production of other types of lattice-tuning semiconductor substrates, including substrates terminating at fully relaxed pure Ge allowing III-V incorporation with silicon. It is also  
15 possible in accordance with the invention to incorporate one or more surfactants, such as antimony for example, in the epitaxial growth process in order to produce even smoother virtual substrate surfaces and lower density threading dislocations by reducing surface energy.

20 Figure 1 shows a long thin stripe of SiGe material 1 which is grown within a confined area between Si oxide walls 2 which surround the SiGe material on four sides. During the growth of the layer of SiGe within this area by epitaxial growth, dislocations 3 form preferentially along the shortest dimension of the area, that is from one long oxide wall towards the other opposite, long oxide wall. These dislocations 3 are  
25 generated at dislocation nucleation sites 4 along one or other of the long oxide walls, as illustrated in each case by a "X" in the figure. This is generally attributed to the ease of dislocation formation at the edge of the growth zone. Where dislocations are formed along the shortest dimension, these dislocations are able to extend to the opposite edge of the zone substantially unhindered. However, dislocations tending to form along the  
30 longest dimension of the zone are quickly blocked by the dislocations formed along the shortest dimension, and thus cannot traverse the entire length of the zone. Such dislocations 5 are shown in Figure 1 as being generated from one end of the zone but

being quickly pinned at pinning locations 6 by the dislocations 3 extending along the shortest dimension.

Consequently the SiGe material in this case can only be relaxed in one direction  
5 by the formation of the dislocations extending along the shortest dimension, whilst  
remaining unrelaxed in the orthogonal direction due to the failure of dislocations to  
form along the longest dimension (although there may be some elastic relaxation if the  
shortest dimension is small enough). Whilst the above described difficulties are  
discussed above in relation to growth of SiGe within a limited area confined by oxide  
10 walls 2, similar problems are found where SiGe is required to be grown within an area  
limited by the area of the substrate surface, for example on top of an etched mesa pillar.

Accordingly, in accordance with a method of the invention for forming a relaxed  
SiGe virtual substrate suitable for growth of strained Si or SiGe active layers and  
15 unstrained III-V semiconductor active layers within which active semiconductor  
devices, such as MOSFETs, may be fabricated, a layer of oxide is grown on a Si  
substrate 10 and is then selectively etched after the area to be etched has been defined,  
for example by the application of a photoresist layer to the oxide layer and the selective  
exposure and development of the photoresist layer to form a photoresist mask. After  
20 etching elongate walls 11 of oxide extend substantially parallel to one another along the  
length of the substrate 10 and are separated by long thin strips 12, as shown at a in  
Figure 2, within which a SiGe layer may subsequently be grown in the manner already  
described above.

25 In the subsequent epitaxial growth process a SiGe layer 13 is selectively grown  
on each long thin strip 12 between the oxide walls 11, as shown at b in Figure 2. Such  
SiGe growth is selective such that there is substantially no growth of SiGe along the top  
of the oxide walls 11. Such selective growth may be effected by chemical vapour  
deposition (CVD).

30

As indicated at c in Figure 2 dislocations 14 are caused to be generated at each  
oxide wall 11 and to extend along the shortest dimension towards the opposite oxide



wall 11. In this manner the SiGe material is caused to relax in the direction of the dislocations 14 which extend over the entire width of the area between the walls 11.

Subsequent to such relaxation, which may be assisted by an annealing step if  
5 required carried out at an elevated temperature in the range of 500 to 1,200°C, epitaxial  
growth of SiGe material is continued until lateral overgrowth of the SiGe material onto  
the top of the oxide walls 11 occurs, as shown at d in Figure 2. Eventually the grown  
areas of SiGe seeded in the areas between the oxide walls 11 will coalesce with each  
other and cover the entire surface of the Si substrate. The SiGe material grown in this  
10 manner may form a single crystalline layer, or alternatively there may be stacking faults  
where the different growth zones coalesce. It is in any case likely that the surface will  
be uneven where the different growth zones meet.

As the growth of the SiGe material continues, the strain in the unrelieved  
15 longitudinal direction is eventually relaxed by the formation of dislocations extending in  
the longitudinal direction which are able to be nucleated from anywhere on the wafer.  
Since such nucleation has a much higher activation energy than nucleation from the  
oxide walls on the sides of the growth zone, the formation of such longitudinal  
dislocations 15 occurs at a much later stage than the formation of the dislocations 14  
20 within the windows defined by the oxide walls 11.

As the longitudinal dislocations 15 are formed at a higher level than the  
dislocations 14 within the windows, the two sets of dislocations 13, 15 do not interact  
with one another and the dislocations may extend over the whole surface of the wafer.  
25 Furthermore, because there is no strain in the SiGe material in a direction orthogonal to  
the outside walls 11, there will be no driving force tending to produce dislocations in  
this direction. Furthermore, since any dislocation interactions are kept to a minimum,  
there are substantially no threading dislocations produced which would otherwise  
terminate at the upper surface of the SiGe material resulting in roughness of the surface.

In this manner a high quality virtual substrate is produced which may be used for the growth of strained Si or SiGe active layers and unstrained III-V semiconductor active layers within which active semiconductor devices may be fabricated.

5           In the above described method the height of the oxide walls 11 may vary from 10 nm to 1,000 nm depending on the Ge composition of the SiGe material, although it would normally be expected to be in the range of 400 nm to 700 nm. The oxide windows may range in width from 2  $\mu\text{m}$  to 100  $\mu\text{m}$  in width, and most likely are from 5  $\mu\text{m}$  to 20  $\mu\text{m}$  in width. The width of the oxide walls 11 is preferably as small as  
10 possible to ensure full lateral overgrowth, and currently the width is likely to be about 1  $\mu\text{m}$ .

          The Ge composition within the SiGe material may be substantially constant through the thickness of the layer, although it would also be possible for the Ge  
15 composition to be graded so that it increases from a first composition at a lower level in the layer to a second, higher composition at a higher level in the layer.

          Various modifications of the above-described method are possible within the scope of the invention. For example, after sufficient growth of the SiGe material has  
20 taken place to provide overgrowth of the tops of the oxide walls 11, an uneven surface 16 may be obtained, as shown at d in Figure 2, and the effect of this may be overcome by a chemo-mechanical polishing (CMP) step to planarise the surface before a final capping layer is grown to obtain the final arrangement shown at e in Figure 2. In a  
25 further modification, an annealing step is applied to ensure full relaxation. Such an annealing step may be effected at any stage in the SiGe growth process, although it is preferably effected after the selective SiGe growth between the oxide walls 11 and before the further growth leading to overgrowth of the oxide walls 11.

          In a further modification, instead of the SiGe material being grown between  
30 oxide walls, the SiGe growth occurs on top of closely spaced mesa pillars defining the growth zones. In this case the isolation between the strips is provided by the trenches

between the pillars, rather than by isolating oxide walls, and the epitaxial growth process may be molecular beam epitaxy (MBE) or CVD.

5 Furthermore the virtual substrate may be epitaxially grown on a patterned silicon wafer or a wafer having a patterned oxide layer such that growth only occurs in selected areas. Thus the fabrication technique may be used to produce a virtual substrate in only one or more selected areas of the chip (as may be required for system-on-a-chip integration) in which enhanced circuit functionality is required, for example.

10 The method of the invention is capable of a wide range of applications, including the provision of a virtual substrate for the growth of strained or relaxed Si, Ge or SiGe layers for fabrication of devices such as bipolar junction transistors (BJT), field effect transistors (FET) and resonance tunnelling diodes (RTD), as well as III-V semiconductor layers for high speed digital interface to CMOS technologies and  
15 optoelectronic applications including light emitting diodes (LEDs) and semiconductor lasers.

**CLAIMS:**

1. A method of forming a lattice-tuning semiconductor substrate, comprising:  
5  
    (a) defining parallel strips of a Si surface by spaced parallel isolating means;  
  
    (b) selectively growing a first SiGe layer on the strips such that first  
dislocations extend preferentially across the first SiGe layer between the isolating  
10 means to relieve the strain in the first SiGe layer in directions transverse to the isolating  
means; and  
  
    (c) growing a second SiGe layer on top of the first SiGe layer to overgrow  
the isolating means such that second dislocations form preferentially within the second  
15 SiGe layer above the isolating means to relieve the strain in the second SiGe layer in  
directions transverse to the first dislocations.
2. A method according to claim 1, wherein the first SiGe layer has a Ge  
composition ratio that is substantially constant within the layer.  
20
3. A method according to claim 1 or 2, wherein the second SiGe layer has a Ge  
composition ratio that is substantially constant within the layer.
4. A method according to claim 1, 2 or 3, wherein at least one of the SiGe layers  
25 has a Ge composition ratio that increases within the layer from a first level to a second  
level greater than the first level.
5. A method according to any preceding claim, wherein at least the first SiGe layer  
is annealed at an elevated temperature in order to substantially fully relieve the strain in  
30 the layer.

6. A method according to claim 5, wherein the growth of the first and second SiGe layers is carried out at a temperature in the range of 350 to 900°C, and the annealing of at least the first SiGe layer is carried out at an elevated temperature in the range of 500 to 1200°C.

5

7. A method according to any one of claims 1 to 6, wherein the first and second SiGe layers are formed by a single continuous growth process.

10

8. A method according to any one of claims 1 to 6, wherein intermediate processing is conducted between the growth of the first SiGe layer and the growth of the second SiGe layer.

15

9. A method according to claim 8, wherein the intermediate processing incorporates a step of annealing the first SiGe layer at an elevated temperature in order to substantially fully relieve the strain in the first SiGe layer.

10. A method according to claim 8 or 9, wherein the intermediate processing step incorporates a chemo-mechanical polishing step.

20

11. A method according to any preceding claim, wherein the first SiGe layer is grown by a selective epitaxial growth process.

12. A method according to claim 11, wherein the epitaxial growth process is chemical vapour deposition (CVD).

25

13. A method according to claim 11, wherein the epitaxial growth process is molecular beam epitaxy (MBE).

30

14. A method according to any preceding claim, wherein the strips of Si oxide have a thickness in the range of 10 nm to 1000 nm, and preferably in the range of 1400 nm to 700 nm.

15. A method according to any preceding claim, wherein the strips of Si oxide have a width in the range of 0.5 nm to 10 nm, and preferably about 1 nm.
16. A method according to any preceding claim, wherein the strips of Si oxide are spaced apart by a distance in the range of 2  $\mu\text{m}$  to 100  $\mu\text{m}$ , and preferably in the range of 5  $\mu\text{m}$  to 20  $\mu\text{m}$ .
17. A method according to any preceding claim, further comprising the step of growing on top of the first and second SiGe layers a strained Si layer within which one or more semiconductor devices are formed.
18. A method according to any preceding claim, wherein the isolating means comprises spaced parallel walls of Si oxide on the Si surface.
19. A method according to any preceding claim, wherein the isolating means comprises spaced parallel trenches in the Si surface.
20. A method of forming a lattice-tuning semiconductor substrate, substantially as hereinbefore described with reference to the accompanying drawings.
21. A lattice-tuning semiconductor substrate formed by a method according to any preceding claim.
22. A lattice-tuning semiconductor substrate substantially as hereinbefore described with reference to the accompanying drawings.

**ABSTRACT****"Formation of Lattice-Tuning Semiconductor Substrates"**

5 A method of forming a lattice-tuning semiconductor substrate comprises the  
steps of defining parallel strips of a Si surface by the provision of spaced parallel oxide  
walls 2 on the surface, selectively growing a first SiGe layer on the strips such that first  
dislocations 3 extend preferentially across the first SiGe layer between the walls 2 to  
relieve the strain in the first SiGe layer in directions transverse to the walls 2, and  
growing a second SiGe layer on top of the first SiGe layer to overgrow the walls 2 such  
10 that second dislocations form preferentially within the second SiGe layer above the  
walls 2 to relieve the strain in the second SiGe layer in directions transverse to the first  
dislocations 3. The dislocations so produced serve to relax the material in two mutually  
transverse directions whilst being spatially separated so that the two sets of dislocations  
cannot interact with one another. Thus the density of threading dislocations and the  
15 surface roughness is greatly reduced, thus enhancing the performance of the virtual  
substrate by decreasing the disruption of the atomic lattice that can lead to scattering of  
electrons in the active devices and degradation of the speed of movement of the  
electrons.

(Figure 1)